

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane
26103-08-2 | DTXSID60448843

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 847 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

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Dichlobenil

Measured: 316

Predicted: 328

Image not found

2,4,5-Trichlorophenol

Measured: 2290

Predicted: 757

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1,2,4-Trichlorobenzene

Measured: 1260

Predicted: 1560

Image not found

1,2,3-Trichlorobenzene

Measured: 2140

Predicted: 1800

Image not found

Benzene, 1-bromo-4-nitro-

Measured: 263

Predicted: 448